METHODS AND DEVICES FOR IDENTIFYING RELATED IONS FROM

CHROMATOGRAPHIC MASS SPECTRAL DATASETS CONTAINING

OVERLAPPING COMPONENTS

5   **RELATED APPLICATIONS**

This application is a continuation-in-part of Attorney Docket No. 10020515-1

US 20040180446

(2003309-0034), U.S. Patent Application No. 10/388,088, filed March 13, 2003 entitled "

Methods and Devices for Identifying Biopolymers Using Mass Spectroscopy", Dean R.

Thompson and Steven M. Fischer, which is incorporated herein by reference in its entirety.

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   BACKGROUND

   Technical Field

   This application is related to mass spectral analysis, and more particularly to

15   *processing mass spectra generated by mass spectral analysis.*

   Description of Related Art

   Mass spectroscopy is a powerful analytical tool that may be used in identifying

unknown compounds as well as their quantities. Mass spectroscopy may also be useful, for

20   example, in elucidating the structure and chemical properties of molecules, and may be used

in connection with organic as well as inorganic substances. The identification of proteins and

other molecules in a complex mixture derived from biological sources may be performed

using mass spectroscopy. A variety of different techniques have been developed for use with

the identification of molecules, such as proteins.

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filtered data may be grouped according to the group vector which results from performing the steps of flowchart 700.

The example display 1400 of Figure 17 represents the reordered m/z rows such that m/z rows in the same group are adjacent. After selecting relevant scan(s) for each group, the corresponding intensities for the selected scans may be obtained from the filtered data set to produce a resulting spectra. In one embodiment as described herein, the scans may be selected by finding the scan or time at which each group maximizes the correlation value by adding the rows of the data matrix for each group and selecting the scan with the maximum intensity value.

The foregoing processing techniques described herein, for example, in connection with flowchart 400, may not be used in instances where there are two or more molecules that elute at the same time and also have the same elution profile. In this instance, the foregoing processing steps are not able to identify the different peptides and properly pair parent (U spectra) with fragments (F spectra), and another processing technique may be used, for example, as described in Attorney Docket No. 10020515-1 (2003309-0034), AGS-00101 US 20040180446 U.S. Patent Application No. 10/388,088 filed March 13, 2003, entitled " Methods and Devices for Identifying Biopolymers Using Mass Spectroscopy", hereinafter referred to as "the Thompson and Fischer disclosure". The processing steps of Thompson and Fischer may be performed on the results produced by processing steps described herein to resolve the parent-fragment pairings in instances where two or more molecules elute at the same time. The Thompson and Fischer disclosure describes a method for gathering structural information for biopolymers in a sample by running the mass spectrometer in the alternating scan mode, as described elsewhere herein, with alternating U and F spectra. Alternating scan